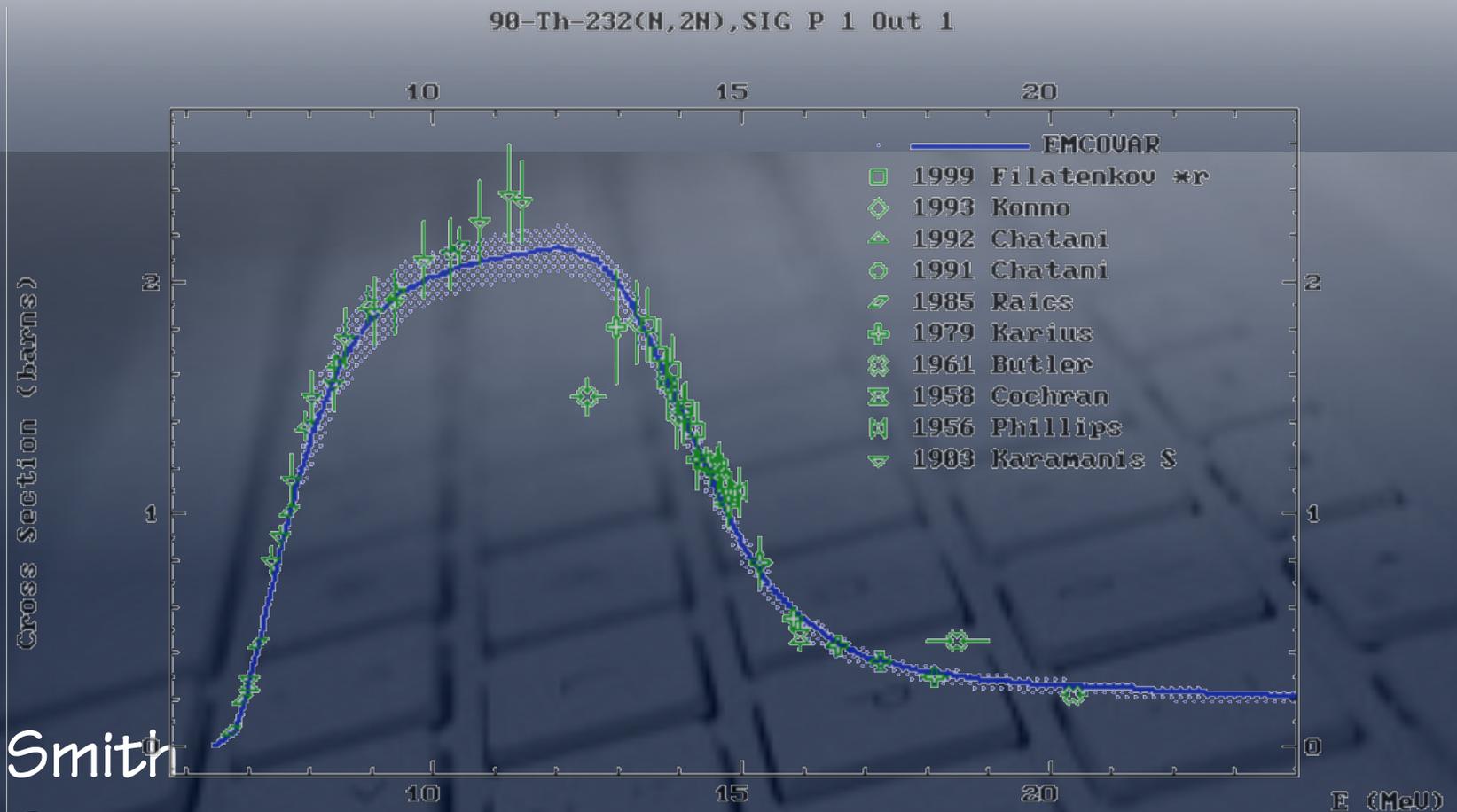


# Software for USNDP



Michael Smith  
Physics Division  
Oak Ridge National Lab  
Oak Ridge, Tennessee

# Motivation

Optical Model parameters  
collection and tools  
*B. Kay, ANL*

Plotting tools for  
nuclear structure  
*R. Casten, Yale*

Collection of theory results  
and database of theory codes  
*A. Brown, MSU*

Access XUNDL and ENSDF  
simultaneously  
*M. Carpenter, ANL*

Digitizing cross sections from  
transfer reactions  
*B. Kay, ANL*

GTNDSE code used to  
search & plot data  
(maintain / develop)  
*M. Allmond, ORNL*

Tools for pre-review of  
manuscripts  
*Multiple attendees*

Generate level schemes  
with Radware  
*M. Carpenter, ANL*

HSCALC tool extracting band  
info from ENSDF (generalize)  
*M. Carpenter, ANL*

Comprehensive inventory of  
existing tools located in one  
place  
*Multiple attendees*

Direct access to databases for  
data extraction  
*M. Carpenter, ANL*

Structure tools and codes  
*A. Brown, MSU*

- Strong need for **new software tools** was **repeatedly expressed** by **researchers** at the Notre Dame Workshop
  - opportunity for researchers to more fully utilize USNDP products
  - many creative ideas, but lack expertise to implement and resources to maintain

# Motivation

## Apply automatic data re-normalization

Users' corrections, help, documentation

Apply corrections

Auto corrections is possible

### Web tools for ENSDF evaluators

by V.Zerkin, IAEA-NDS, 2011-2016, ver.2016-06-28  
Upload your ENSDF dataset and run remotely ENSDF codes: FMTCHK, chk\_ENSDF, PREPRO, XPQCHK, ALPHAD, GTOL, Brctc, BrctcMixing, GABS, LOGFT, PANDORA, RADLST, RULER, NDS PUB, etc.

Evaluator: Viktor  
Working area: 21  
Session: 21

Use existing ENSDF file:  No file chosen

or ENSDF text. Examples:  Test input:          1-5 152 aa 177Lu 235Pa

184AU 184HG EC DECAY 2005SA40,1994Ib01,1978E1010NDS 201002  
184AU H TYP=FULSAUT=CORAL M. BAGLINS=CIT=NDS 111,275 (2010)SCUT=1-Oct-2009\$  
184AU D PARENT T: 30.6 S 3 (1972F112), 30.9 S 3 (1994a23).  
184AU D 32.5 S 10 (1970Ha18); from 5535A(T). 32.0 S 10 (1969Ha03).  
184AU D WEIGHTED AVERAGE: 30.87 S 26.  
184AU c Others: 1975Ho03, 1971Hu02, 1969Ha03 (observed 157g and 237g).  
184AU c 2005SA40: mass-separated (+184)Hg source from fragmentation of molten  
184AU c Pb target by 600 MeV or 1 GeV protons; Ge(Li) and Si(Li) detectors,  
184AU c high resolution 180" magnetic spectrograph; measured E<sub>g</sub>, I<sub>g</sub>,  
184AU c E(ce), I(ce). Additional sources from (+148)Sm(+40)Ar,X); planar Ge  
184AU c (F<sub>WH</sub>=0.9 keV at 122 keV) for E<sub>g</sub><1 MeV; two HPGe detectors (F<sub>WH</sub>  
184AU c [22.3 keV at 1.3 MeV) for E<sub>g</sub><1.3 MeV; measured x-g-t and lg-t  
184AU c events which were dimensional to provide prompt-, total- and delayed-  
184AU c coincidence bidimensional matrices (60 ns or 100 ns time windows).  
184AU c Supersedes 2003Ib2Z; see also 1994Ib01.  
184AU c 1994Ib01: mass separated source from bombardment of (+148)Sm by 185 MeV  
184AU c (+40)Ar ions; He-jet transport, iodine aerosol; two HPGe coaxial

Login: Viktor 2016/08/24 15:49:06 161.5.6.220:Austria Access level=2

#	Area	ENSDF file	Files	Created	
1.1	tmp16	Viktor 184Au.ens	8	2016/08/22 09:01:54	Viktor 161.5.6.223:Austria <input type="button" value="continue"/>
2.1	tmp20	Nikola 123Ba.ens	7	2016/08/23 15:08:07	Nikola 140.105.22.76:Italy <input type="button" value="continue"/>

Web Design and Programming: Viktor Zerkin, NDS, International Atomic Energy Agency (V.Zerkin@iaea.org)  
Last updated: 08/24/2016 17:49:40

Useful links:  
• NSDD  
• NuDat2  
• LiveChart  
• ENSDF  
- web-retrieval  
- manual  
- programs  
- data archive  
• XUNDL  
- web-retrieval  
- data archive  
• x4pdf-nr  
• x4pdf-all

Copy/Paste/Edit your ENSDF data file or put Web link

Continue your previous session

• Strong need for **new software tools** has also been requested by **SOME evaluators**

- opportunity for evaluators to benefit from recent software innovations to increase productivity, accuracy, reliability ...
- some new tools are being developed (JAVA NDS)
- IAEA has moved in this direction (MyENSDF, X4 tools ...)

# Categories of Software

	Visualization	Data Diving	Workflow	Executable
Access Codes				
Science Codes and Pipelines				
Evaluator Tools				

- Many different types of software used in nuclear science
- Matrix of code categories suggests **gains** from **parallel development of multiple tools** by reusing code components

# Meeting the Needs

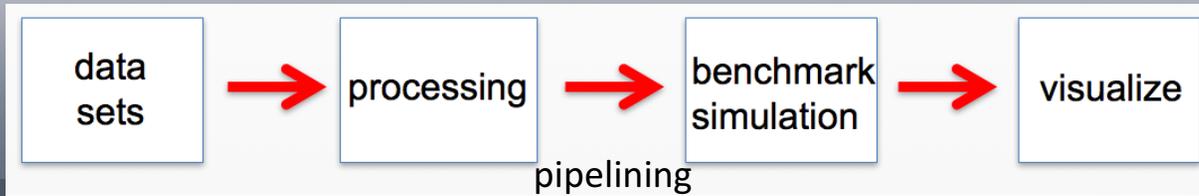
- “Software business as usual” **will not meet community requests** for new tools or realize possible gains in productivity, ease-of-use ...
  - Software has a lower priority than evaluation work
  - Software development requires different skill set
  - Any proposal for incremental software work within the USNDP will compete for funds with evaluations
- Significant progress will require a **new approach**

# New Data Software Project

- *Suggested Key Features*

- *finite performance period (such as 3 years)*
- *focus on projects rated highest priority*
- *realistic milestones and deliverables*
- *well managed effort with project controls*
- *separate funding*
- *not replace / conflict with ongoing work*
- *involve professional level coders advised by data experts*

# New Data Software Project

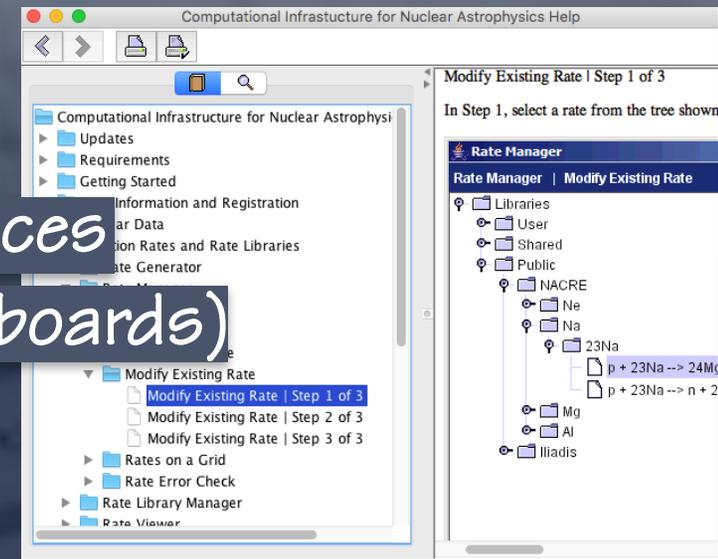


To select the rate of interest, select a method below and click *Continue*.

- Select reaction from the Chart of the Nuclides
- Select reaction from a tree
- Enter Z and A values for each reactant and product

User chooses entry method

- Things to do
  - query Users for projects
  - prioritize projects
  - query Users for features / preferences
  - pay attention to interfaces (storyboards)
  - emphasize pipelining when possible
  - include heavy documentation
  - provide multiple views / paths / approaches
  - provide in-system help / guides / manuals
  - provide upgrade paths



Online help

# New Data Software Project

- Things to avoid ... don't
  - develop tools that aren't needed
  - duplicate efforts
  - focus on new formats (too controversial)
  - work with proprietary architectures
  - assume all Users want the same features
  - keep codes proprietary

# New Data Software Project

- More things to avoid ... don't
  - build for a single platform
  - exclusively use old paradigms (downloads)
  - ignore cloud-based solutions
  - develop in a vacuum (ignore other products)
  - assume others will develop tools we request
  - assume that one solution will work for all

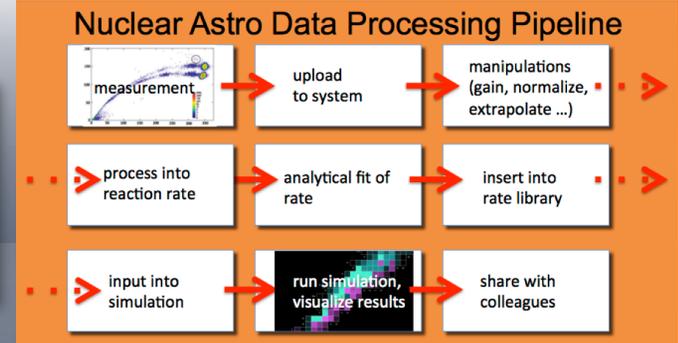
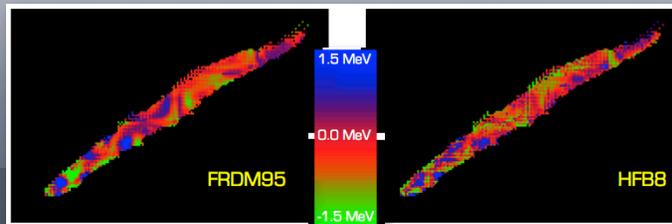
# Pioneering Efforts at ORNL

NUCASTRODATA.ORG

**BIG BANG ONLINE**



nuclearmasses.org



- **Computational Infrastructure for Nuclear Astrophysics**
  - Cloud-based solution offering unique capabilities in the field that span the range from nuclear data to reaction rates to simulations
  - Enables users to upload, manipulate, manage, visualize, share nuclear information and complex simulations
- **Nuclear Mass Toolkit**
  - Cloud-based solution offering unique comparisons between mass data sets from evaluations, compilations, experiments, and theory
- **Big Bang Nucleosynthesis**
  - Users can set up and run custom simulations of element creation in the early universe
- **Cloud Computing**
  - Plenary talk at ND2010 on Cloud Computing for Nuclear Data envisioned a new paradigm for data activities
  - NDC3.net established to host future work
- **Bellerophon\***
  - Huge expansion of CINA for supernova simulations on ORNL Supercomputers
- **BEAM\***
  - Expansion of Bellerophon for materials science research at ORNL, spanning desktops, clusters, supercomputers with drag-and-drop queueing and file transfers

\* Led by Eric Lingerfelt

# Pioneering Efforts at ORNL



## PRODUCT CATALOG

### Product Catalog - Periodic Table

Please click on a purple box to see the products available for that element.  
If you would like an isotope product that is not listed,  
you can make a request by clicking here.

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
		Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr		



## PRODUCT CATALOG

### Silver

[Back](#)

Isotope	Natural abundance (atom %)	Isotopic enrichment (atom %)	Request a Quote
Ag-107	51.35	>99	<a href="#">Request a Quote for This Ag-107 Product</a>
Ag-109	48.65	>99	<a href="#">Request a Quote for This Ag-109 Product</a>

**PRODUCT FORM**

Inventory Form	metal
Alternate Form	chloride, nitrate, acetate

## PRODUCT CATALOG

### Product Catalog - Process Online Quote Into Online Order

Step 2 - Review the selected online quote below.

Online Quote Confirmation Number	100005					
Name of Online Quote Creator	Eric Lingerfelt					
Online Quote Creation Date	2014-04-03 08:25:59					
Isotope	Inventory Form	Enrichment	Batch Number	Amount (mg)	Price per mg of element (U.S. \$)	Total Price (U.S. \$)
W-184	Oxide	95.060	56401-A	700	1.71	1,197.00
S-34	Elemental	85.590	150190	600	61.34	36,804.00

## Mar FY2012 Online Snapshot



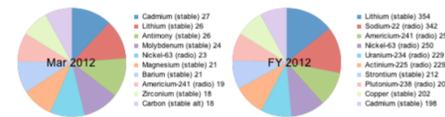
### Product Hits

Total Hits for FY 2012: 17800

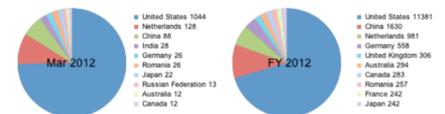
Total Hits for Mar 2012: 1456



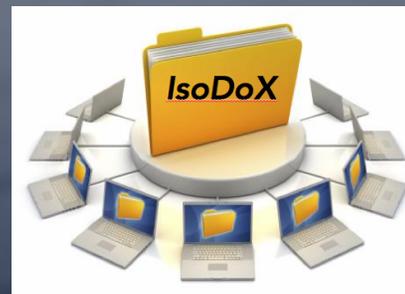
### Top 10 Products



### Top 10 Countries



Timestamp: 2012-03-27 12:14:20



- **Isotopes.gov**

- Modernized DOE's isotope program IT infrastructure
- Cloud solution features catalog with multiple entry methods, ordering, preferred customers "one click" ordering features, top-notch security, tool kit and interface custom designed for Isotope Business Office, custom permissions, associated expansive website ...
- Time-saving "snapshots" of data activities can do a weeks work with a few clicks ... duplicates functions of excel, powerpoint, pdf exports
- Done as **separate DOE Project** with milestones & project controls

Software for USNDP

Michael Smith



# Path Forward

- identify sponsors
- gather interested parties
- discuss possible projects
- solicit project suggestions from community
- prioritize projects
- write and submit proposal